5-2000

The Design of a Chemical Plant Using HYSYS Simulation Program

Michael Randolph Vaughan
University of Tennessee - Knoxville

Appendix D - UNIVERSITY HONORS PROGRAM
SENIOR PROJECT - APPROVAL

Name: Michael Vaughan

College: Engineering Department: Chemical

Faculty Mentor: Dr. Charles Moore

PROJECT TITLE: The Design of a Chemical Plant Using HYSYS Simulation Program

I have reviewed this completed senior honors thesis with this student and certify that it is a project commensurate with honors level undergraduate research in this field.

Signed: Charles F. Moore, Faculty Mentor

Date: 5/8/2000

Comments (Optional):

University Honors Senior Project
Spring 2000

The Design of a Chemical Plant Using HYSYS Simulation Program

by:

Michael Vaughan

Faculty Advisor: Dr. Charles Moore

Honors Director: Dr. Thomas Broadhead

Department of Chemical Engineering
University Honors Program
University of Tennessee
Knoxville, TN 37996

Table of Contents

List of Figures

Introduction and Background

The purpose of this project was to learn about the computer simulation tool, HYSYS, and how engineers can use it. The overall objective was to design a basic chemical plant with a reactor, distillation column and recycle stream. Another aspect of the study was to use HYSYS to develop a general understanding of chemical plant control and process control concepts.

HYSYS is an advance process simulation environment for the process industries developed by Hyprotech, a business unit of AEA Technology Engineering Software. AEA Technology Engineering Software is a leading developer and supplier of best in class software solutions serving the Process, Automotive, Aerospace and Manufacturing industries. As an integrated simulation environment, HYSYS allows engineers to develop a single process model that can be utilized for many applications, ranging from conceptual design to on-line functions. HYSYS is a powerful software tool that can be used by engineers to design plants and processes, optimize production, and enhance decision-making. It also provides the means for engineers and operators to gain an understanding of their processes, as well as, practice plant operation and make process modifications in a safe and reliable environment.

This tool is unique in that it is the only commercially available simulation environment designed for complete user customization. This enables companies to create a seamless combination of proprietary unit operations, reactions and property packages, as well as allowing interaction with other applications and software programs. Particular technologies that HYSYS offers include conceptual design, steady-state design, dynamic design, and real-time simulation. To accomplish these tasks, HYSYS utilizes accurate thermodynamic and reaction models, complete physical property libraries, and many unit operations and utilities, such as reactors, distillation columns, and heat exchangers.

To actually build a plant model in HYSYS, a flowsheet is designed by adding various unit operations (all the different equipment and processes used in a chemical plant) and the appropriate process streams, which represent liquids or gases flowing from one unit operation to the next. Streams are also added to represent heating or cooling streams that are found in all chemical plants. HYSYS operates inside an event driven graphical environment that is combined with an interactive approach to modeling and a

non-sequential modular solution algorithm. A PFD user interface is the easiest way to design the entire flowsheet graphically, allowing one to install operations and streams and then connecting them with the mouse. Once all the unit operations and streams are connected properly, HYSYS automatically performs all the necessary calculations and produces all the results for each operation and stream, i.e., the performance and characteristics.

Basic Plant Design

Setting Up Hypothetical Components

The project at hand focused on designing a basic chemical plant composed of one reactor, a distillation column and a recycle stream. A previous plant had been built using an old simulation tool on a Macintosh based system called DynaMac. The main task was to take the design of that plant and convert it to a HYSYS model. The plant was to be set up using four hypothetical components, termed A, B, R, and S. This allowed for more generality, so that the same model could be used for varying purposes in the future by professor Moore. The hypothetical components were related by the following two reactions:

$$A + B \rightarrow R \quad (1)$$

$$2B \rightarrow S \quad (2)$$

where A and B are the feed reactants, R is the desired product, and S is an undesired side product. The goal of the plant is to produce the desired product R in a reactor. This involves optimizing the production of R, minimizing the production of S, and then separating the R from the other components in a distillation column to obtain purified R in the product stream.

In order to set up hypothetical components in HYSYS, it was decided to use the clone component function of HYSYS. This allows the user to clone a real component and then modify its properties as desired. Therefore, the first step done was to find real components that had similar properties to those given in the DynaMac design, in particular, components with the same molecular weight. The real components used in the HYSYS set up were water, acetaldehyde, glycol, and ethyl acetate, with molecular weights of 18, 44, 62, and 88, respectively. These real components were cloned to the hypothetical components A, B, R, and S, respectively. Much time was then spent converting the physical properties of the hypothetical components in HYSYS to correlate with those given from DynaMac. The physical properties from the DynaMac program were given in English units and are shown in Appendix A. Some of the basic properties included molecular weight, liquid density, vapor pressure, heat of vaporization, and ideal gas heat capacity and are shown in equation form, as most of the properties are

temperature dependent. Unfortunately, HYSYS uses slightly different properties and property definitions to define its components, making it difficult to convert between programs. The major modifications that were necessary were the vapor pressures of each component, as the DynaMac vapor pressures deviated from the real components used in HYSYS. For example, the component S was modified to have no vapor pressure. Also, several of the B and R properties were changed to be the same as A, as indicated from the DynaMac specifications. The hypothetical HYSYS component properties are shown in Appendix B.

Designing the Distillation Column

It was decided that the first unit operation to be designed would be the distillation column, as HYSYS is flexible in the set-up of a plant model. When designing in steady-state mode, one can begin at any location in the model because HYSYS uses a non-sequential modular calculation structure. This means that the unit operations and streams in HYSYS are calculated automatically. The results of any calculation are automatically passed throughout the flowsheet to whichever streams and operations are affected by the change. When calculations are complete, one can be sure that all possible calculations have been performed.

Based on reaction 1, one mole of the desired product, R, is produced from one mole each of feed reactants A and B. Also, reaction 2 shows that one mole of the undesired product, S, is produced by reacting 2 moles of B together. Therefore, in order to minimize the occurrence of S, it was deemed necessary to feed an excess amount of A to the system. This would help ensure that all of the B would be used up in the first reaction, with very little being left over to form any S. As such, it was first assumed that a mixture of mostly A, some R, and very little S and B would be the product stream coming from the reactor. Hence, this mixture would then need to be separated in order to obtain the desired product, R, in the product stream. This was accomplished with the distillation column unit operation.

A distillation column is used to separate components of a mixture based on their differences in boiling points or their relative volatilities. The lower boiling substances are vaporized in the column and leave the column out the top, while the higher boiling or

heavier components remain in the liquid phase and are removed out the bottom of the distillation column. The relative volatilities are related to the vapor pressure and the molecular weight of each component. Since the feed reactants A and B have a lower molecular weight and higher vapor pressure, they will be taken out the top of the distillation column in the distillate stream. The products, R and S, have lower vapor pressures and will be removed out the bottom of the column in the bottoms product stream.

The basic distillation column consists of the column itself, a reboiler, and a condenser. The reboiler is attached to the bottom of the column and is used to heat up and vaporize the contents, whereas the condenser collects the vapors from the top of the column and condenses them back into a liquid before they move on. Part of the liquid stream from the condenser is usually returned to the top of the distillation column as a reflux stream to enhance the separation capability of the column. Figure 1 below shows a diagram of a basic distillation column including a reboiler and condenser, and is representative of the one designed in HYSYS.

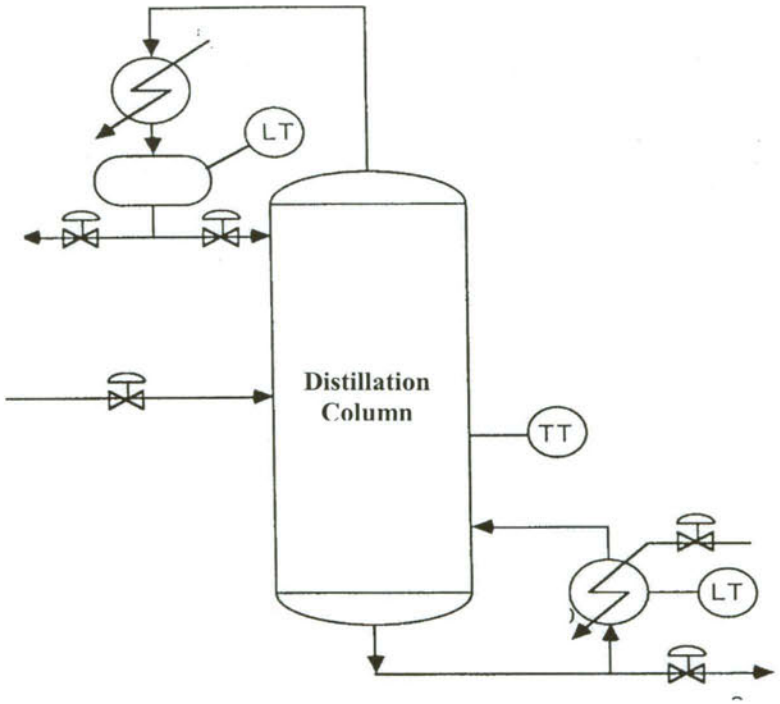

Figure 1: Diagram of a Basic Distillation Column

In HYSYS, there are many specifications and parameters to set when designing a distillation column. Besides the reboiler and condenser, one must set the number of trays inside the column (trays are used to obtain equilibrium between the liquid and vapor phases and thus increase the separation of the components), feed composition, feed stream location, column pressure, etc. HYSYS is capable of using several different solving methods and algorithms to simulate a real distillation column, so those must be chosen too. Along with the basic specifications, HYSYS allows one to base your column on a wide range of design variables, enabling one to achieve the desired results and see how the distillation column performs under various conditions. Usually, one to three design variables must be specified by the user, and they can include variables such as the distillate rate, reflux ratio (ratio of the amount of liquid stream leaving the condenser that is going back to the column to the amount that is going elsewhere), bottoms rate, component fractions in the top or bottom of the column, heat duty (amount of heat being supplied by the reboiler), etc.

From the discussion above about using an excess amount of A in the system, the feed stream compositions were first set to be approximately 85% A, 13.5% R, 1% S and 0.5% B. The molar flow rate of the feed stream was set at 100 kgmol/hr, with a temperature of 25 ^{o}C and pressure of 120 kPa. The distillation column was set up with 20 trays and the feed stream entering at tray #10. The pressure was set to vary linearly from 107 kPa at the top to 127 kPa at the bottom of the column. The solving methods and options were left in the default mode. Next, in order to simulate the operation of the distillation column, two design variables had to be set by the user. It was first decided to base the column operation on the distillate rate and the reflux ratio. Initial values of 80 kgmol/hr for the distillate rate and 2.00 for the reflux ratio were chosen. Now, HYSYS had all the necessary information to begin calculations and determine if the column could actually operate under the given conditions. If the conditions and solving methods were feasible, the column would have converged to a real solution. If a real solution is met, the non-user-specified variables are set by HYSYS, including the compositions of the distillate and bottoms streams. Therefore, one can see how well the distillation column is performing at separating the components. For the initial guess, the column did not converge, which is usually the case when first building a distillation column. Upon

further modification of the design variable values, the column continued to run into problems and not converge. Several other design variables, such as the heat duty going to the reboiler and the component mole fraction of A in the vapor leaving the top of the column, were also chosen to run the column around. However, nothing seemed to work quite right. Then, the solving method was changed from HYSIM Inside-Out to Modified HYSIM Inside-Out and the damping factor (used to help the calculations) was changed from fixed to adaptive. Finally, specifying a distillate rate of 85.5 kgmol/hr and a reflux ratio of 2.00, the column converged and reached a real solution. The distillate or overhead stream contained 99.4% A, 0.06% B, and no R or S. The bottoms product stream consisted of 93.1% R and 6.9% S, with no A or B. Thus, the column effectively achieved the goal of separating the feed reactants from the products. A printout of all the distillation column specifications and results from HYSYS is shown in Appendix D.

Designing the Reactor

The next step in the plant model was to design the reactor in order to simulate the two reactions taking place. Since the two reactions are based on kinetic principles, it was decided to model the reactions with a Continuous Stirred Tank Reactor or CSTR. This kinetic reactor calculates the conversion of the reactants based on the rates of the reactions taking place. In a CSTR, the inlet stream is assumed to be perfectly mixed with the contents of the reactor, so that the outlet stream is identical in composition and temperature to that of the reactor contents. It was also assumed that the reactions were liquid phase only, so that the rate was only dependent on the temperature of the reactor and the inventory of the reactants.

Like the distillation column, several specifications for the CSTR were necessary to be set by the user. First, the reactions had to be defined in the reaction package of HYSYS. The stoichiometric coefficients for each reaction were first entered and then from the information given from the DynaMac model, the reaction rate parameters were inputted. The reaction rate for the first reaction is given by the following equation:

$$\text{Rate Rxn1} = k_1 * [C_A] * [C_B] \qquad (3)$$

where k_1 is the forward specific reaction rate constant and C_A and C_B are the concentrations of each component in the reactor. The specific reaction rate constant is a function of temperature and is defined by the Arrhenius equation shown below:

$$k = A \exp[-E/RT] \quad (4)$$

where A is the pre-exponential factor, E is the activation energy, R is the gas law constant and T is the temperature of the reaction. From the DynaMac information given, A is $5.0x10^4$ and E is 5000 for reaction 1. These values were plugged into HYSYS, along with values of zero for the reverse reaction. HYSYS then automatically calculated the heat of reaction based on the properties of the hypothetical components. For the second reaction, the reaction rate is given by:

$$\text{Rate Rxn2} = k_2*[C_B]^2 \quad (5)$$

From the DynaMac model, A equals $2.0x10^{13}$ and E equals 20000 for k_2. The DynaMac and HYSYS reaction specifications are shown in Appendix A and Appendix C, respectively. Note that the heats of reactions for both reactions were calculated by HYSYS to be significantly different than the values given by the DynaMac model. This could be due to the differing unit values of several of the parameters. For the actual HYSYS model, these discrepancies altered the results slightly, but did not hinder the overall objectives, and further evaluation was not deemed necessary.

After the reactions were set up, the actual reactor was implemented into the flowsheet ahead of the distillation column. One feed stream was connected along with two product streams, a liquid stream and a vapor stream. Since the feed stream is a liquid and the reactions are both liquid phase reactions, no vapor is produced in the reactor. So, the vapor product stream has nothing in it and is hidden in the flowsheet. An energy stream was also necessary to be added. The reactants, A and B, were to enter the system separately, so they were combined in a small unit operation called a mixer in HYSYS. This operation simply performed a material and energy balance on the two entering feed streams to give a single outlet stream. This outlet stream, consisting of A and B, was the feed stream to the CSTR. Again, it was necessary to have an excess amount of A feeding the reactor, so that all of the B is consumed in the first reaction and not the second. Therefore, the A feed was initially set at 100 kgmol/hr with a temperature of 25 $^{\circ}$C and a pressure of 101 kPa. The B feed was set at 10 kgmol/hr with the same temperature and

pressure as the A feed. The feed stream to the reactor then consisted of 90.9% A and 9.1% B, with a molar flow rate of 110 kgmol/hr, a temperature of 25 °C, and a pressure of 101 kPa.

For the reactor, the vessel volume and pressure drop across the reactor were set at 2.0 m^3 and 0.0 kPa, respectively. The function of the energy stream could either be set to heating or cooling, and in this case, was set to heating with a user-specified value of $2.0x10^5$ kJ/hr. Finally, the vapor-phase fraction of the CSTR liquid stream product was specified as zero, and HYSYS was ready to simulate real operation. Compared to the distillation column, HYSYS did not have as many problems finding a solution for the reactor. For this first CSTR model, HYSYS calculated that almost all the 10 kgmol/hr of B entering the reactor were converted into the desired product, R. Only $1.1x10^{-5}$ kgmol/hr of S were produced. This produced a product stream consisting essentially of only 90% A and 10% R. This specifications and results for this first model of the CSTR are shown in Appendix E.

Combining the CSTR and Distillation Column and Adding a Recycle Stream

After the CSTR was working, the product stream was connected to the feed stream going to the distillation column. Doing this altered the conditions of the stream going to the distillation column and thus the operation and performance of the column. Several modifications were necessary in order to make the distillation column converge. The component mole fraction of A in the vapor leaving the top of the distillation column was used as a design variable instead of the distillate rate, although the column probably would have converged either way. Because it was desired to have very little R leaving the top of the reactor, using the component fraction of A out the top as a design variable enabled the column to better achieve this goal.

The final step in the basic plant design was to add a recycle stream, so that the excess A being taken out the top of the distillation column could be recovered and sent back to the reactor feed stream. This helps minimize the amount of fresh A needed in the reactor feed stream, and thus the cost of the reactants. HYSYS has a specific recycle operation and is used when downstream material streams are fed back upstream in the process. The recycle operation solves the flowsheet by performing calculations that are

passed back to the original streams without any inconsistencies. The inlet of the recycle operation was set as the distillate stream from the distillation column and the outlet of the recycle operation was termed the A Recycle stream. This A Recycle stream was then added as another feed stream to the mixer at the front of the plant. Now, the mixer had three streams entering it with one outlet stream, still going to the feed of the CSTR. After numerous calculations, HYSYS eventually reached a solution for the entire plant. This solution was only one of many possible solutions, based on the amount of A that could be built up in the system. Now that a large amount of A was entering the CSTR from the recycle stream, the fresh A and B feed streams were modified to both have molar flow rates of 70 kgmol/hr. The CSTR and distillation column were recalculated with the new conditions and their specifications and results are shown in Appendix F. Note that almost all of the 70 kgmol/hr of B entering the system is converted to R and that all 70 kgmol/hr of R produced is separated out the bottom of the distillation column. The HYSYS process flowsheet for the final version of the basic plant model is shown in Figure 2 on the next page.

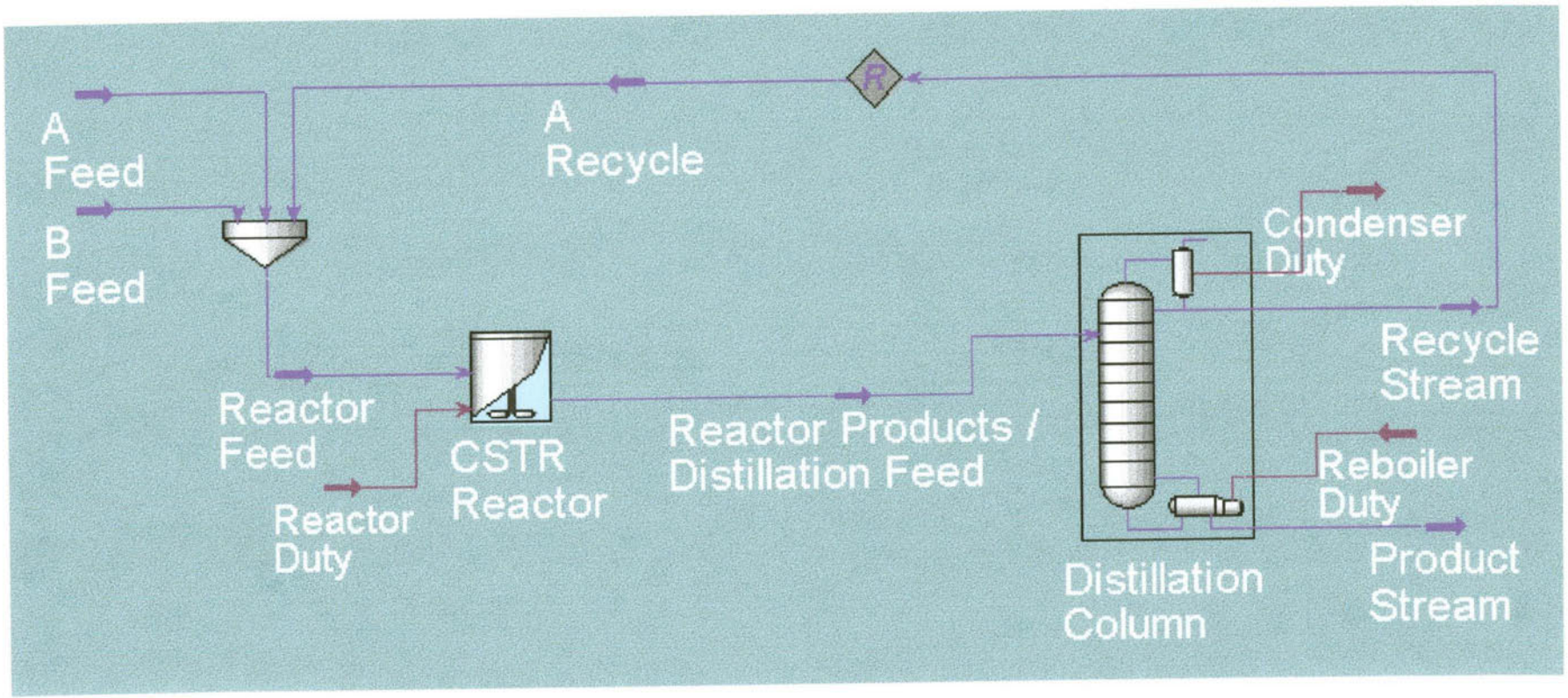

Figure 2: Schematic of HYSYS Flowsheet for Basic Plant Model

Process Control

Background on Process Control in HYSYS

Now that the basic plant had been designed in steady-state mode, showing how each unit operation performs under normal conditions, it was desired to see how the plant would behave under dynamic conditions, since this is really how chemical plants operate. To do this, one must become familiar with the concepts of process control. The field of process control encompasses the basic principles most useful when applied to many systems encountered by chemical engineers, such as chemical reactors, heat exchangers, and mass transfer equipment. With an understanding of transient behavior of physical systems, engineers can better design processes and plants that perform well in the real and continually changing world. A major component of process control is the concept of feedback control. Feedback control is central to most automation systems that monitor a process and adjust some variables to maintain the system at or near desired conditions. Feedback control makes use of an output of a system to influence an input to the same system. When feedback is employed to reduce the magnitude of the difference between the actual and desired values of a variable, it is termed "negative feedback" (Marlin, 1995).

HYSYS uses proportional-integral-derivative (PID) controllers to control the flow through a valve in order to achieve a desired set point for a process variable, the variable one wishes to maintain at a certain value. The proportional part of the controller makes the control action proportional to the error signal, which is the difference between the desired process variable set point and the actual process variable value. So, as the error increases, the adjustment to the manipulated variable, which is the variable that is altered in order to positively affect the process variable, is increased. The proportionality constant is called the controller gain, usually termed K. The integral part of the PID controller compensates for the shortcomings of the proportional mode by itself, by continually adjusting the manipulated variable until the magnitude of the error is reduced to zero. Finally, the derivative mode does not affect the final steady-state value of the error, but provides a rapid correction based on the rate of change of the controlled

variable. Each of the parts in PID control has a parameter associated with it that can be tuned by the user for better control performance.

These PID controllers are used by HYSYS only in the dynamic mode and can be used in several different manners, most commonly for feedback control. The set-up of a PID controller in HYSYS involves three sections: connections, parameters, and tuning. The connections involve the process variable source and the output or manipulated variable. Here, the minimum and maximum range of the control valve is also set. The parameters are used to set the range for the process variable, the PV minimum and PV maximum. This range is used in calculating the output, based on the current error. This must be set in order for the controller to operate. Another parameter is the controller action, which defines how the valve will be manipulated (opening or closing) when the PV is above or below the desired set point. The last parameter is the controller mode, which can be one of six different modes. When the mode is off, the controller takes no action. If it is set to manual, the user can set the output for the controller directly, as a percentage of the valve span. In auto mode, the output is calculated based on the controller equation and the currently set values for the gain, integral time, and derivative time. With ramping SP mode, the desired final set point is set along with the time required to ramp the set point from its current value to the final value. In cascaded SP mode, the current controller is a slave controller, with its set point being set as the output from a master controller. Finally, auto-tuning mode causes the controller to set up a limit cycle, opening and closing the valve by ten percent on either side of the current set point. The tuning section of the PID controller set-up in HYSYS is where the user specifies the values for each parameter of the controller, the proportional gain constant (Ki), the integral time (Ti), and the derivative time (Td).

Developing a Basic Control Strategy in HYSYS

To begin setting up a basic control strategy for the plant, it was decided to first add a PID controller to help control the operation of the distillation column. The temperature profile of the column was examined, and it was determined to use the temperature of the system at the 5^{th} tray location as the process variable to control around. This particular temperature location was chosen because the largest change in

temperature for the column occurred around this tray, i.e., this is where most of the separation was taking place. Next, the manipulated variable was set to be the reboiler duty, which is the amount of heat in the form of steam that is added to the bottom of the column. The reboiler duty has a direct affect on the temperature profile of the distillation column. Since the current value of the temperature at tray 5 was 130 °C, the PV minimum and maximum were set to 80 and 180 °C, respectively. The reboiler had a current value of 6.0×10^7 kJ/hr, so the control valve range was set between 0.0 and 8.0×10^7 kJ/hr. The controller action was set to reverse and the controller mode was set to automatic. Additionally, the tuning parameters were set with the controller gain initially as 1.0, the integral time as 30 minutes, and the derivative time as zero. With the controller specified, HYSYS was placed in dynamic mode. Once in dynamic mode, HYSYS uses an integrator to run all the necessary calculations to simulate the real-world operation of the plant. Unfortunately, HYSYS was not able to run in dynamic mode with the way the chemical plant was set up. HYSYS was having major difficulties simulating the operation of the CSTR in dynamic mode. This greatly limited the amount of study that could be done for this project.

However, in order to perform a few control studies, the design of the plant was altered to remove the CTSR. A simple hold up tank was put in its place, which acted as a tank to collect material streams without any reaction taking place. The feed stream to the hold up tank was set to be similar to what was coming out of the CSTR in the basic plant model (it included mostly A, some R, and very little S). Therefore, the distillation column would still be operating under similar conditions. HYSYS was finally able to run in dynamic mode with this new simplified plant model. The PID had to be updated under the new conditions. The largest temperature change in the distillation column was at stage 11 now, so this was the location of the process variable. With the PID set, the integrator was started and the controller began operating in automatic mode. The performance of the controller was examined using the Databook tool in HYSYS and in particular the Stripcharts, which showed each variable of the PID controller: the process variable, manipulated variable, and the control output. A few disturbances were simulated to study the performance of the controller and determine if the tuning parameters needed to be adjusted. One example of a step change to the system involved

altering the temperature of the feed stream going into the distillation column from 58 °C to approximately 66 °C. The PID controller quickly reacted in order to maintain the temperature of the process variable (tray 11 temperature) close to its set point of 110 °C. The output to the manipulated variable, which was the reboiler duty, was slightly decreased, which simulated closing the valve and thus decreasing the amount of heat added to the column by the reboiler. The PID controller performed well, in that the actual temperature of tray 11 remained very close to the set point. The controller gain of 1.0 and the integral time of 30 minutes were therefore deemed effective. An example of this test is shown in Figure 3 on the next page. Note that the output for the manipulated variable is on a different scale than temperature; it is on a percent scale from 0 to 100%.

The next step in the process control strategy was to add a temperature controller on the hold up tank, in order to have control over the temperature of the material streams that lead to the distillation column. A similar PID controller as before was installed, with the hold up tank temperature as the process variable and the tank duty as the manipulated variable. After a few tests involving disturbances to the hold up tank, the tuning parameters were adjusted to 1.5 for the gain and 60 minutes for the integral time. Figure 4 shows a schematic of the HYSYS flowsheet after the two temperature PID controllers had been added. The controllers are represented as circles with a line through them. The arrows indicate that the controller is obtaining information from the process variable and then sending the output to the manipulated variable. The two PID temperature controller specification sheets are shown in Appendix G.

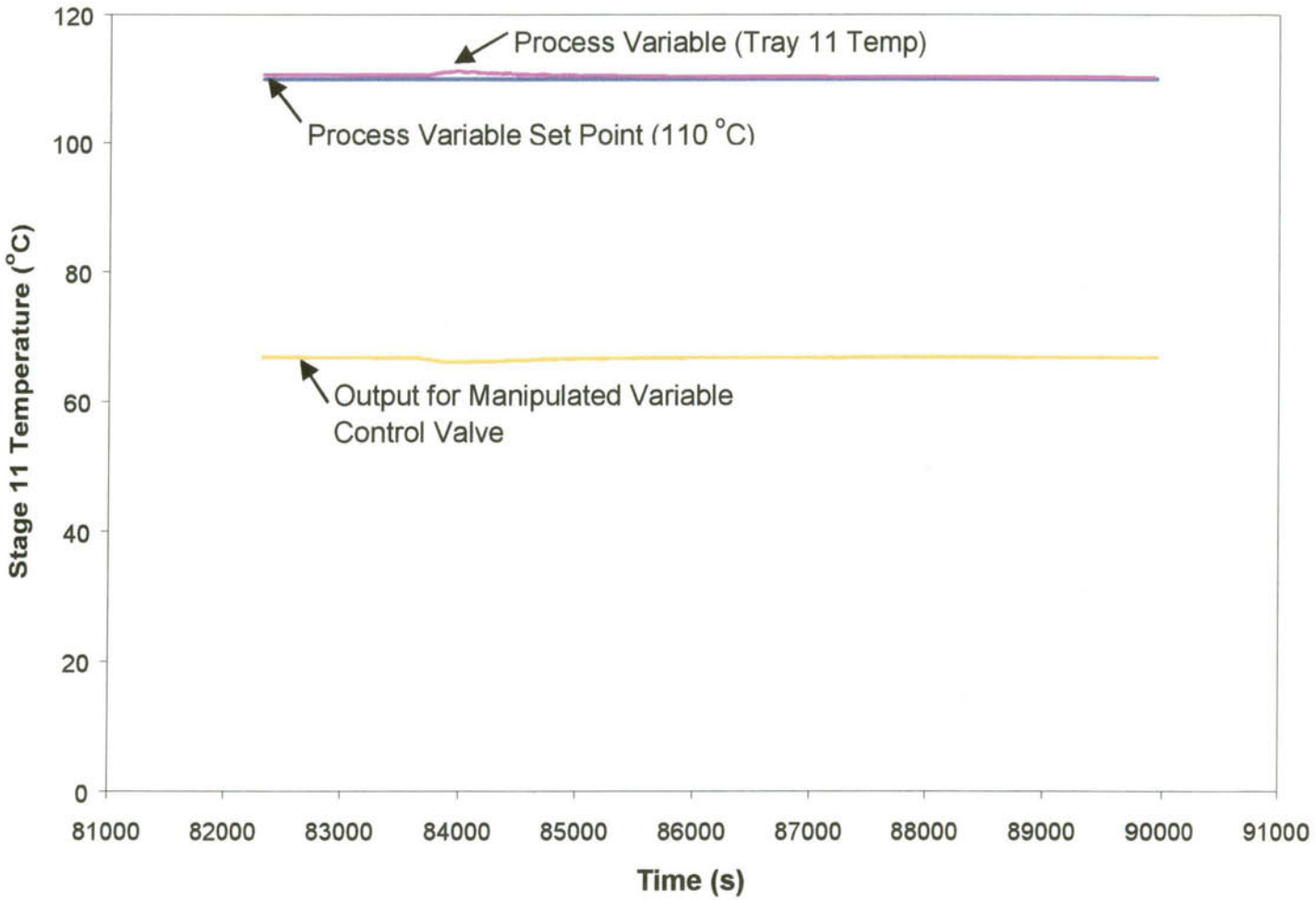

Figure 3: Example of PID Controller Performance for Distillation Column

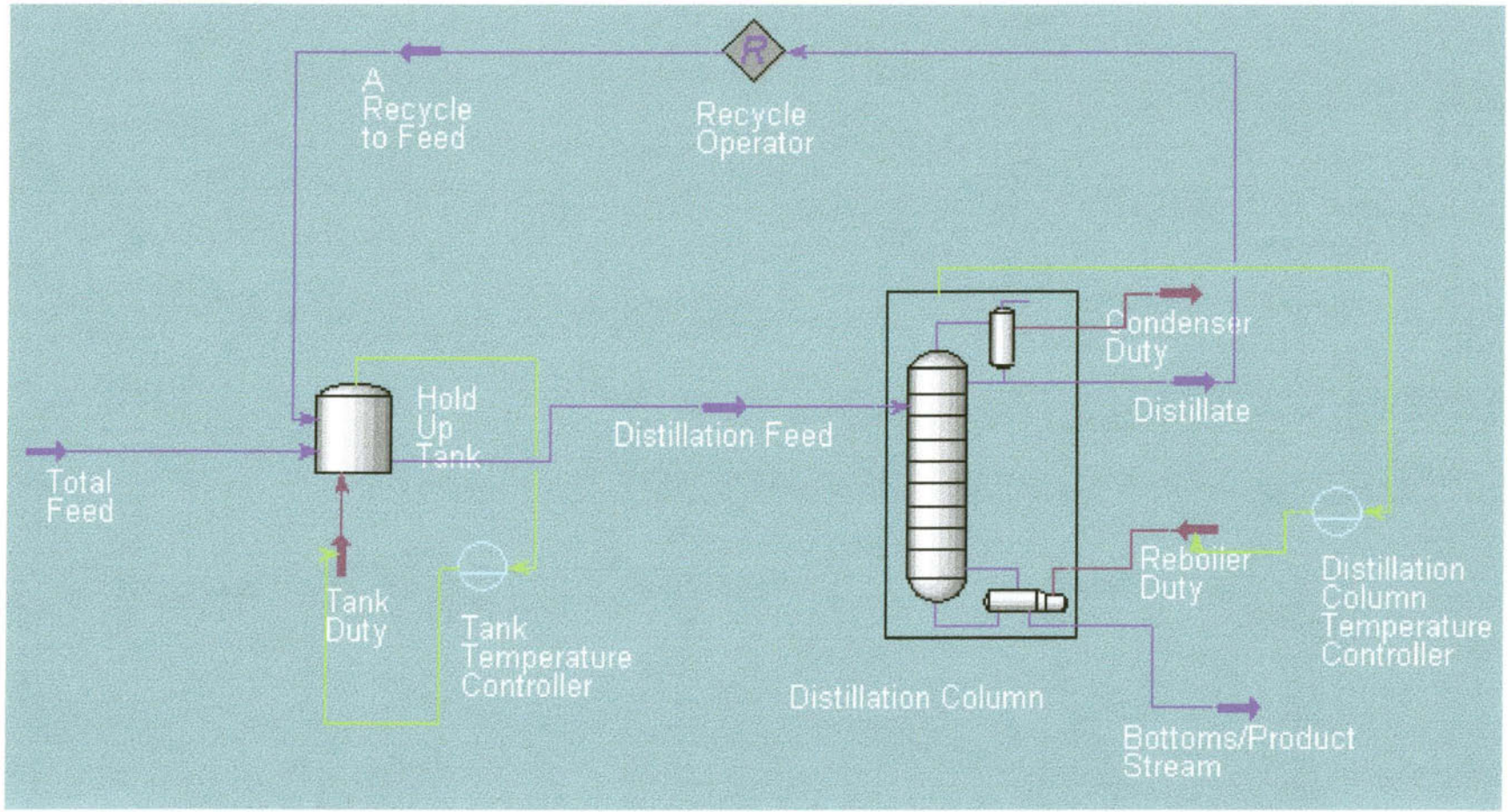

Figure 4: Schematic of HYSYS Flowsheet with Two PID Temperature Controllers

Further control studies were attempted, but with only limited results. It was desired to simulate the effect of building up or depleting the amount of excess A that was in the system. This involved looking at how much A was in the recycle stream, as well as how much A was entering the system. If more A was entering the system than necessary, the amount of A in the recycle would go up. Eventually, this build up would decrease the efficiency of the plant. Therefore, in order to alleviate this potential problem, a new material stream was added to the distillation column in order to remove small amounts of A from the system. This was done by adding a side draw stream to the distillation column near the top of the column where the contents are almost pure A. With this side stream, a more complicated control system was necessary to control the amount of A in the system. First, the ratio of the molar flow rate of A entering the system to the molar flow rate of A leaving the system through the side draw was calculated using the Spreadsheet function of HYSYS. The spreadsheet takes the molar feed rates of the A entering the system and leaving the system as inputs and then calculates their ratio as an output available to a controller. Next, a PID controller was added that essentially operated as a ratio controller. It was set up with the ratio from the spreadsheet as its process variable and the A removal flow rate as its output or manipulated variable. The control action was direct, the gain was 1.0, and the integral time was 30 minutes. HYSYS was set in dynamic mode and the integrator was started. The control system was operable and a few studies were conducted. The set point of the ratio controller was altered, which changed the amount of A leaving the system through the side draw. When the ratio was decreased, more A was leaving the system than was entering, and thus, the amount of A in the recycle began to decrease. Conversely, when the ratio was increased, more A was being fed to the system, and the A recycle went up. The user could employ this method to achieve a desired amount of A in the system, as well as, simulate disturbances to the system in terms of the A feed rate. A schematic of the HYSYS flowsheet including the spreadsheet and ratio controller is shown in Figure 5. Appendix G has the specification sheet for the PID ratio controller.

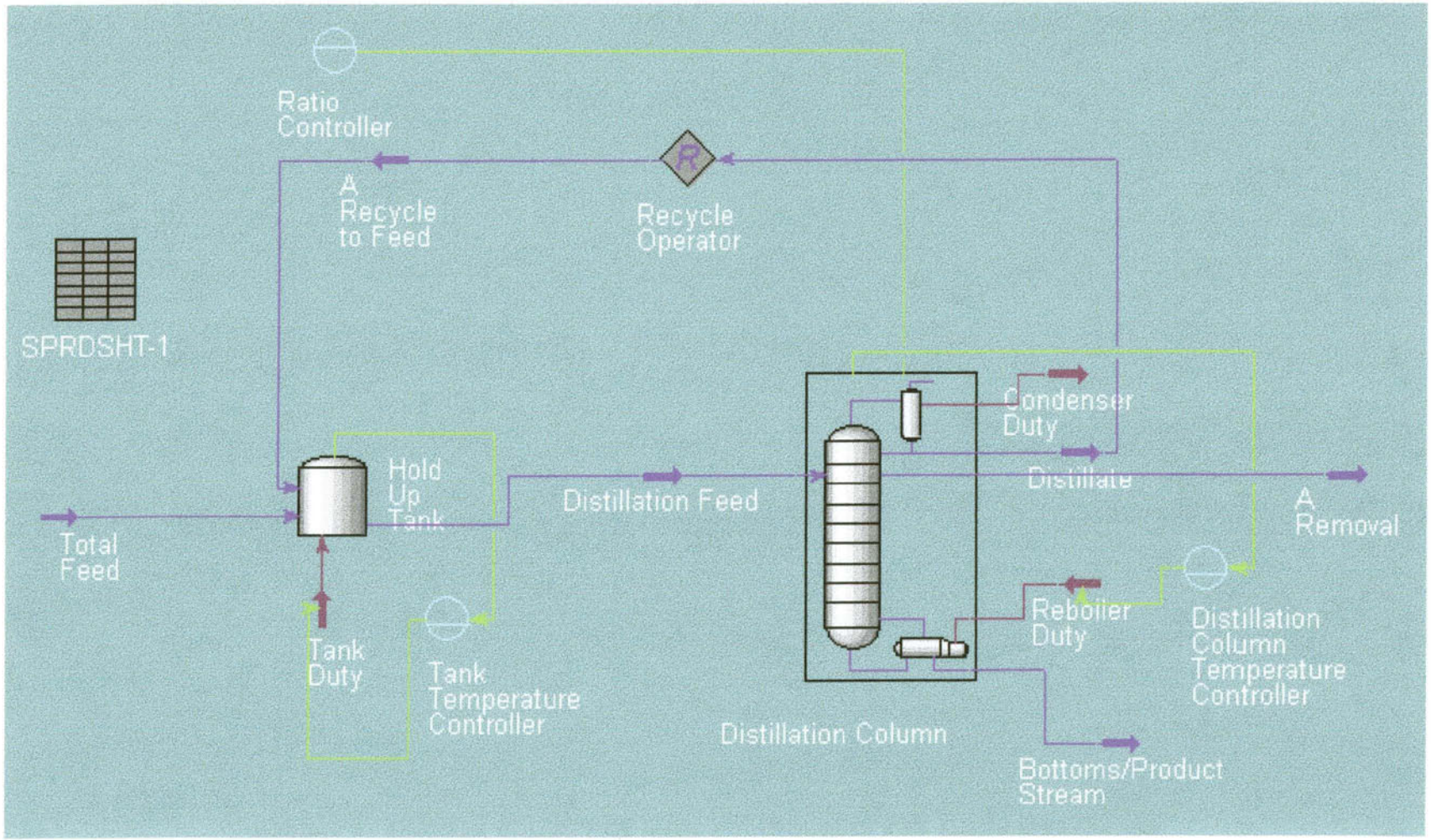

Figure 5: HYSYS Schematic with Spreadsheet and Ratio Controller

Conclusions

From this project, a good working knowledge of HYSYS and its operation was realized. An understanding of the benefits, as well as, the idiosyncrasies of HYSYS was also obtained through a lot of trial and error and reading the help menus and manuals. The overall objective of designing a basic chemical plant was accomplished. The plant model was set up in steady-state mode, and included a CSTR reactor, a distillation column, and a recycle stream. The CSTR reactor simulated two reactions taking place between the four hypothetical components, A, B, R, and S.

$$A + B \rightarrow R \quad (1)$$

$$2B \rightarrow S \quad (2)$$

An excess amount of A was fed to the reactor, so that all the B was used up in the first reaction to produce the desired product, R, and none of the undesired product, S. The distillation column then simulated the separation of the liquid mixture in order to obtain purified R in the product stream. A recycle stream was added to the plant model, so that the excess A separated in the distillation column could be recovered and returned to the feed to the CSTR reactor.

The basic concepts of process control were then studied and a basic control strategy was implemented in several steps to the HYSYS plant model. The first step involved adding two PID temperature controllers to control the operation of the distillation column and the hold up tank, which took the place of the CSTR for the process control studies. HYSYS was run in dynamic mode to simulate real plant processes and operation. The controllers successfully operated by maintaining the process variables at their desired set points even when disturbances were inflicted on the system. The second control strategy implemented involved a ratio controller to simulate the control of the amount of excess A in the system. This controller was used with a new A removal side dray stream, to increase or decrease the amount of A in the system. More control studies were attempted, but time did not permit the analysis to be completed.

Reference List

Marlin, Thomas E., *Process Control*, McGraw-Hill, Inc., New York, 1995.

All other information obtained from HYSYS program and help menus.

Appendix A: DynaMac Physical Properties and Reaction Specifications

Property	*Units*	*Eqn Type*	*Ai*	*Bi*	*Ci*	*Di*
Component A						
Molecular Weight	Lb/LbMol		18.01			
Liq Molar Volume	cc/gmol		18.8			
Liquid Density	Lb/CuFt	100	62.44	-6.03E-03	-2.16E-04	
Vapor Pressure	Torr	110	19	-3841	228	
Heat of Vaporization	Btu/Lb	100	1057	-0.823	-3.54E-04	-5.28E-06
Liquid Heat Capacity	Btu/Lb*F	100	1.003	-2.11E-04	2.26E-06	2.59E-09
Ideal Gas Heat Capacity	Btu/Lb*F	100	0.33	-2.19E-03	2.57E-06	
Component B						
Molecular Weight	Lb/LbMol		44			
Liq Molar Volume	cc/gmol		18.8			
Liquid Density	Lb/CuFt	100	62.44	-6.03E-03	-2.16E-04	
Vapor Pressure	Torr	110	17.36	-3841	228	
Heat of Vaporization	Btu/Lb	100	1057	-0.823	-3.54E-04	-5.28E-06
Liquid Heat Capacity	Btu/Lb*F	100	1.003	-2.11E-04	2.26E-06	2.59E-09
Ideal Gas Heat Capacity	Btu/Lb*F	100	0.33	-2.19E-03	2.57E-06	
Component R						
Molecular Weight	Lb/LbMol		62			
Liq Molar Volume	cc/gmol		18.8			
Liquid Density	Lb/CuFt	100	62.44	-6.03E-03	-2.16E-04	
Vapor Pressure	Torr	110	16.5	-3841	228	
Heat of Vaporization	Btu/Lb	100	1057	-0.823	-3.54E-04	-5.28E-06
Liquid Heat Capacity	Btu/Lb*F	100	1.003	-2.11E-04	2.26E-06	2.59E-09
Ideal Gas Heat Capacity	Btu/Lb*F	100	0.33	-2.19E-03	2.57E-06	
Component S						
Molecular Weight	Lb/LbMol		88			
Liq Molar Volume	cc/gmol		18.8			
Liquid Density	Lb/CuFt	100	62.44	-6.03E-03	-2.16E-04	
Liquid Heat Capacity	Btu/Lb*F	100	1.003	-2.11E-04	2.26E-06	2.59E-09
Non-Volatile -- no vapor pressure, heat of vaporization, IG heat capacity						

Equation Types

100 X =Ai +Bi(T) + Ci(T^2) + Di(T^3)

110 X = exp (Ai + Bi/(T + Ci))

DynaMac Reaction Specifications

Reaction 1

1 Comp A (L) + 1 Comp B (L) ----> 1 Comp R (L)

RATEfor = Kfor [Comp A] ^1 [Comp B] ^1

Kfor = 4.9651e4 * EXP [- 5000. /(1.987*(T+273.))]
Krev = 0.0000E+00 * EXP [- 0.0000E+00/(1.987*(T+273.))]

Heat of Reaction -20000 BTU/mol B reacted

Reaction 2

2 Comp B (L) ----> 1 Comp S (L)

RATEfor = Kfor [Comp B] ^2

Kfor = 2.0e+13 * EXP [- 20000. /(1.987*(T+273.))]
Krev = 0.0000E+00 * EXP [- 0.0000E+00/(1.987*(T+273.))]

Heat of Reaction -50000

HYSYS Pure Component Specsheet — Senior Project Version 7.hsc

A*

Identification

Family / Class	Chemical Formula	ID Number	Group Name	CAS Number
Miscellaneous	H2O	20000	HypoGroup1	---

UNIFAC Structure

H2O

User ID Tags

Tag Number	Tag Text

Critical/Base Properties

Base Properties			Critical Properties		
Molecular Weight		18.02	Temperature	(C)	374.1
Normal Boiling Pt	(C)	100.0	Pressure	(kPa)	2.212e+04
Std Liq Density	(kg/m3)	998.0	Volume	(m3/kgmole)	0.05710
			Acentricity		0.3440

Additional Point Properties

Thermodynamic and Physical Properties			Property Package Molecular Properties		
Dipole Moment		1.800	PRSV - Kappa		-0.1942
Radius of Gyration		0.6150	KD Group Parameter		---
COSTALD (SRK) Acentricity		-0.6544	ZJ EOS Parameter		---
COSTALD Volume	(m3/kgmole)	0.04357	GS/CS - Solubility Parameter		23.49
Viscosity Coefficient A		-0.8678	GS/CS - Molar Volume	(m3/kgmole)	0.01413
Viscosity Coefficient B		-1.107	GS/CS - Acentricity		0.3440
Cavett Heat of Vap Coeff A		0.2657	UNIQUAC - R		0.9200
Cavett Heat of Vap Coeff B		---	UNIQUAC - Q		1.400
Heat of Formation (25C)	(kJ/kgmole)	-2.410e+05	Wilson Molar Volume	(m3/kgmole)	0.01788
Heat of Combustion (25C)	(kJ/kgmole)	0.0000	CN Solubility		---
Enthalpy Basis Offset	(kJ/kgmole)	-2.509e+05	CN Molar Volume	(m3/kgmole)	---

Temperature Dependent Properties

		Vapour Enthalpy	Vapour Pressure	Gibbs Free Energy
Minimum Temperature	(C)	-270.0	1.850 *	25.00
Maximum Temperature	(C)	-270.0	1.850 *	25.00
Coefficient Name		IdealH Coefficient	Antoine Coefficient	Gibbs Free Coefficient
a		-5.730	65.93 *	-2.417e+05
b		1.914	-7228. *	41.74
c		-0.0003957	0.0000 *	0.007428
d		8.762e-07	-7.177 *	0.0000
e		-4.951e-10	9.500e-06 *	0.0000
f		1.038e-13	2.000 *	0.0000
g		1.000	0.0000 *	0.0000
h		0.0000	0.0000 *	0.0000
i		0.0000	0.0000 *	0.0000
j		0.0000	0.0000 *	0.0000

User Properties

ID	Name	Value

Remarks:

* Specified by user.

HYSYS Pure Component Specsheet — Senior Project Version 7.hsc

B*

Identification

Family / Class	Chemical Formula	ID Number	Group Name	CAS Number
Aldehyde	C2H4O	20004	HypoGroup4	---

UNIFAC Structure

CH3 CHO

User ID Tags

Tag Number	Tag Text

Critical/Base Properties

Base Properties			Critical Properties		
Molecular Weight		44.05	Temperature	(C)	187.9
Normal Boiling Pt	(C)	19.85	Pressure	(kPa)	5570.
Std Liq Density	(kg/m3)	998.0 *	Volume	(m3/kgmole)	0.1540
			Acentricity		0.3030

Additional Point Properties

Thermodynamic and Physical Properties			Property Package Molecular Properties		
Dipole Moment		2.500	PRSV - Kappa		1.000
Radius of Gyration		2.083	KD Group Parameter		---
COSTALD (SRK) Acentricity		0.2647	ZJ EOS Parameter		---
COSTALD Volume	(m3/kgmole)	0.1531	GS/CS - Solubility Parameter		9.552
Viscosity Coefficient A		-0.1492	GS/CS - Molar Volume	(m3/kgmole)	0.05702
Viscosity Coefficient B		-0.3733	GS/CS - Acentricity		0.3030
Cavett Heat of Vap Coeff A		0.2706	UNIQUAC - R		1.899
Cavett Heat of Vap Coeff B		---	UNIQUAC - Q		1.796
Heat of Formation (25C)	(kJ/kgmole)	-1.644e+05	Wilson Molar Volume	(m3/kgmole)	0.01788 *
Heat of Combustion (25C)	(kJ/kgmole)	-1.105e+06	CN Solubility		---
Enthalpy Basis Offset	(kJ/kgmole)	-1.886e+05	CN Molar Volume	(m3/kgmole)	---

Temperature Dependent Properties

		Vapour Enthalpy	Vapour Pressure	Gibbs Free Energy
Minimum Temperature	(C)	-270.0 *	-0.1500 *	25.00 *
Maximum Temperature	(C)	-270.0 *	-0.1500 *	25.00 *
Coefficient Name		IdealH Coefficient	Antoine Coefficient	Gibbs Free Coefficient
a		-5.730 *	37.27 *	-2.417e+05 *
b		1.915 *	-4073. *	41.74 *
c		-0.0003957 *	-80.00 *	0.007428 *
d		8.762e-07 *	-3.362 *	0.0000 *
e		-4.951e-10 *	3.815e-06 *	0.0000 *
f		1.038e-13 *	2.000 *	0.0000 *
g		1.000 *	0.0000 *	0.0000 *
h		0.0000 *	0.0000 *	0.0000 *
i		0.0000 *	0.0000 *	0.0000 *
j		0.0000 *	0.0000 *	0.0000 *

User Properties

ID	Name	Value

Remarks:

* Specified by user.

HYSYS Pure Component Specsheet — Senior Project Version 7.hsc

R*

Identification

Family / Class	Chemical Formula	ID Number	Group Name	CAS Number
Alcohol	C2H6O2	20002	HypoGroup2	---

UNIFAC Structure
(CH2OH)2

User ID Tags

Tag Number	Tag Text

Critical/Base Properties

Base Properties			Critical Properties		
Molecular Weight		62.07	Temperature	(C)	428.8
Normal Boiling Pt	(C)	197.2	Pressure	(kPa)	6515.
Std Liq Density	(kg/m3)	998.0 *	Volume	(m3/kgmole)	0.1860
			Acentricity		0.5600

Additional Point Properties

Thermodynamic and Physical Properties			Property Package Molecular Properties		
Dipole Moment		2.200	PRSV - Kappa		-1.000
Radius of Gyration		2.564	KD Group Parameter		---
COSTALD (SRK) Acentricity		1.228	ZJ EOS Parameter		---
COSTALD Volume	(m3/kgmole)	0.2120	GS/CS - Solubility Parameter		13.53
Viscosity Coefficient A		-0.5527	GS/CS - Molar Volume	(m3/kgmole)	0.06331
Viscosity Coefficient B		-1.448	GS/CS - Acentricity		0.5600
Cavett Heat of Vap Coeff A		0.2462	UNIQUAC - R		2.409
Cavett Heat of Vap Coeff B		---	UNIQUAC - Q		2.248
Heat of Formation (25C)	(kJ/kgmole)	-3.896e+05	Wilson Molar Volume	(m3/kgmole)	0.01788 *
Heat of Combustion (25C)	(kJ/kgmole)	-1.658e+06	CN Solubility		---
Enthalpy Basis Offset	(kJ/kgmole)	-4.237e+05	CN Molar Volume	(m3/kgmole)	---

Temperature Dependent Properties

		Vapour Enthalpy	Vapour Pressure	Gibbs Free Energy
Minimum Temperature	(C)	-270.0 *	58.85 *	25.00 *
Maximum Temperature	(C)	-270.0 *	58.85 *	25.00 *
Coefficient Name		IdealH Coefficient	Antoine Coefficient	Gibbs Free Coefficient
a		-5.730 *	57.94 *	-2.417e+05 *
b		1.915 *	-8861. *	41.74 *
c		-0.0003957 *	37.50 *	0.007428 *
d		8.762e-07 *	-5.717 *	0.0000 *
e		-4.951e-10 *	3.108e-06 *	0.0000 *
f		1.038e-13 *	2.000 *	0.0000 *
g		1.000 *	0.0000 *	0.0000 *
h		0.0000 *	0.0000 *	0.0000 *
i		0.0000 *	0.0000 *	0.0000 *
j		0.0000 *	0.0000 *	0.0000 *

User Properties

ID	Name	Value

Remarks:

* Specified by user.

HYSYS Pure Component Specsheet — Senior Project Version 7.hsc

S*

Identification

Family / Class	Chemical Formula	ID Number	Group Name	CAS Number
Ester	C4H8O2	20003	HypoGroup3	---

UNIFAC Structure
CH3 CH2 CH3COO

User ID Tags

Tag Number	Tag Text

Critical/Base Properties

Base Properties			Critical Properties		
Molecular Weight		88.11	Temperature	(C)	250.1
Normal Boiling Pt	(C)	77.15	Pressure	(kPa)	3820.
Std Liq Density	(kg/m3)	998.0 *	Volume	(m3/kgmole)	0.2860
			Acentricity		0.3620

Additional Point Properties

Thermodynamic and Physical Properties			Property Package Molecular Properties		
Dipole Moment		1.900	PRSV - Kappa		-1.000
Radius of Gyration		3.468	KD Group Parameter		---
COSTALD (SRK) Acentricity		0.3595	ZJ EOS Parameter		---
COSTALD Volume	(m3/kgmole)	0.2853	GS/CS - Solubility Parameter		8.589
Viscosity Coefficient A		0.03730	GS/CS - Molar Volume	(m3/kgmole)	0.09889
Viscosity Coefficient B		-0.2201	GS/CS - Acentricity		0.3620
Cavett Heat of Vap Coeff A		0.2608	UNIQUAC - R		3.479
Cavett Heat of Vap Coeff B		---	UNIQUAC - Q		3.116
Heat of Formation (25C)	(kJ/kgmole)	-4.432e+05	Wilson Molar Volume	(m3/kgmole)	0.01788 *
Heat of Combustion (25C)	(kJ/kgmole)	-2.063e+06	CN Solubility		---
Enthalpy Basis Offset	(kJ/kgmole)	-4.432e+05	CN Molar Volume	(m3/kgmole)	---

Temperature Dependent Properties

		Vapour Enthalpy	Vapour Pressure	Gibbs Free Energy
Minimum Temperature	(C)	-270.0 *	77.15 *	25.00
Maximum Temperature	(C)	-270.0 *	250.1 *	25.00
Coefficient Name		IdealH Coefficient	Antoine Coefficient	Gibbs Free Coefficient
a		0.0000 *	86.49 *	-4.449e+05
b		0.0000 *	-7931. *	384.4
c		0.0000 *	0.0000 *	0.02961
d		0.0000 *	-10.25 *	0.0000
e		0.0000 *	-2.000 *	0.0000
f		0.0000 *	2.000 *	0.0000
g		0.0000 *	0.0000 *	0.0000
h		0.0000 *	0.0000 *	0.0000
i		0.0000 *	0.0000 *	0.0000
j		0.0000 *	0.0000 *	0.0000

User Properties

ID	Name	Value

Remarks:

* Specified by user.

Appendix C: HYSYS Reaction Specifications

HYSYS Kinetic Reaction Specsheet for Project Version 3 with reactor.hsc

Rxn-1

Stoichiometry and Rate Info

Component	Molecular Weight	Stoich Coeff	Forward Order	Reverse Order
A*	18.02	-1.000 *	1.000	0.0000
B*	44.05	-1.000 *	1.000	0.0000
R*	62.07	1.000 *	0.0000	1.000

Balance Error : 0.0000

Reaction Heat : 1.580e+04 kJ/kgmole

Reaction Basis

Basis	Base Component	Rxn Phase	Min. Temp (C)	Max. Temp (C)
Molar Concn	A*	LiquidPhase	-273.1	3000.

Parameters

Forward Reaction		Reverse Reaction	
A : 4.965e+04	*	A' : 0.0000	*
E : 1.163e+04	*	E' : 0.0000	*

Remarks:

* Specified by user.

HYSYS Kinetic Reaction Specsheet for Project Version 3 with reactor.hsc

Rxn-2

Stoichiometry and Rate Info

Component	Molecular Weight	Stoich Coeff	Forward Order	Reverse Order
B*	44.05	-2.000 *	2.000	0.0000
S*	88.11	1.000 *	0.0000	1.000

Balance Error : 0.0000

Reaction Heat : -5.720e+04 kJ/kgmole

Reaction Basis

Basis	Base Component	Rxn Phase	Min. Temp (C)	Max. Temp (C)
Molar Concn	B*	LiquidPhase	-273.1	3000.

Parameters

Forward Reaction		Reverse Reaction	
A : 2.000e+13	*	A' : 0.0000	*
E : 4.652e+04	*	E' : 0.0000	*

Remarks:

* Specified by user.

HYSYS Column Specsheet — Senior Project Trial-dist only.hsc

Distillation Column @Main

Inlet			Outlet		
NAME	STAGE	FROM OPER	NAME	STAGE	TO OPER
Q-101	Reboiler		Q-100	Condenser	
1	10__Main TS		2	Condenser	
			3	Reboiler	
			** New **		

General Parameters

Sub-Flow Sheet:	Distillation Column (COL1)	Number of Stages:	20 *

Column Solving Algorithm: Modified HYSIM Inside-Out

Solving Options		Acceleration Parameters	
Maximum Iterations:	5000. *	Accelerate K Value & H Model Parameters:	Off
Equilibrium Error Tolerance:	1.000e-05 *		
Heat/Spec Error Tolerance:	0.0005000 *		
Save Solutions as Initial Estimate:	On		
Super Critical Handling Model:	Simple K		
Trace Level:	Low		
Init from Ideal K's:	Off	**Damping Parameters**	
Initial Estimate Generator Parameters		Azeotrope Check:	Off
Iterative IEG (Good for Chemicals):	Off	Adaptive Initial Damping Factor:	0.5227 *
		Adaptive Damping Period:	10
		Update Initial Damping Factor:	Off

Specifications Summary

	Specified Value	Current Value	Wt. Error	Wt. Tol.	Abs. Tol.	Active	Estimate
Distillate Rate	85.50 kgmole/h *	85.50 kgmole/h	1.315e-08	0.01000 *	1.000 kgmole/h *	On	On
Reflux Ratio	2.000 *	2.000	-3.331e-15	0.01000 *	0.01000 *	On	On
Reflux Rate	171.0 kgmole/h *	171.0 kgmole/h	0.0000	0.01000 *	1.000 kgmole/h *	Off	On
Btms Prod Rate	14.50 kgmole/h *	14.50 kgmole/h	-1.477e-06	0.01000 *	1.000 kgmole/h *	Off	On
Comp Fraction A in Con	---	0.9975	---	0.01000 *	0.001000 *	Off	On
Reboiler Duty	---	1.145e+07 kJ/h	---	0.01000 *	10.00 kJ/h *	Off	On

Column Specification Details

Distillate Rate

Stream:	2	Flow Basis:	Molar

Reflux Ratio

Stage:	Condenser	Flow Basis:	Molar	Liquid Specification:	Light

Reflux Rate

Stage:	Condenser	Flow Basis:	Molar	Liquid Specification:	Light

Btms Prod Rate

Stream:	3	Flow Basis:	Molar

Comp Fraction A in Cond

Stage:	Condenser	Flow Basis:	Mole Fraction	Phase:	Vapour
Components:		A*			

Reboiler Duty

Energy Stream:	Q-101

Remarks:

* Specified by user.

HYSYS Column Specsheet — Senior Project Trial-dist only.hsc

Distillation Column @Main

Sub-Flowsheet

Feed Streams			Product Streams		
Internal Stream	External Stream	Transfer Basis	Internal Stream	External Stream	Transfer Basis
Q-101	Q-101 @Main	None Req'd	Q-100	Q-100 @Main	None Req'd
1	Distillation Feed @Main	T-P Flash	2	Recycle Stream @Main	T-P Flash
			3	Product Stream @Main	T-P Flash
			** New **		

Tray Summary

Flow Basis: Molar Reflux Ratio: 2.000

	Temp. (C)	Pressure (kPa)	Liquid (kgmole/h)	Vapour (kgmole/h)	Feeds (kgmole/h)		Draws (kgmole/h)		Duties (kJ/h)
Condenser	81.72	107.0	171.0	---	---	Q	85.50	L	-1.066e+07
1 Main TS	81.81	107.0	171.6	256.5					---
2 Main TS	82.18	108.1	172.5	257.1					---
3 Main TS	82.61	109.1	173.9	258.0					---
4 Main TS	83.13	110.2	175.9	259.4					---
5 Main TS	83.77	111.2	178.7	261.4					---
6 Main TS	84.62	112.3	182.1	264.2					---
7 Main TS	86.09	113.3	183.2	267.6					---
8 Main TS	90.81	114.4	166.5	268.7					---
9 Main TS	106.7	115.4	132.9	252.0					---
10 Main TS	127.3	116.5	213.1	218.4	100.0	L			---
11 Main TS	149.4	117.5	219.6	198.6					---
12 Main TS	153.1	118.6	221.6	205.1					---
13 Main TS	153.7	119.6	221.8	207.1					---
14 Main TS	154.0	120.7	222.0	207.3					---
15 Main TS	154.3	121.7	222.1	207.5					---
16 Main TS	154.6	122.8	222.2	207.6					---
17 Main TS	154.9	123.8	222.3	207.7					---
18 Main TS	155.2	124.9	222.4	207.8					---
19 Main TS	155.5	125.9	222.5	207.9					---
20 Main TS	155.7	127.0	221.7	208.0					---
Reboiler	158.0	127.0	---	207.2	---	Q	14.50	L	1.145e+07

Profile Estimates

	Temperature (C)	Net Liquid (kgmole/h)	Net Vapour (kgmole/h)
Condenser	81.72	256.5	2.603e-11
1 Main TS	81.81	171.6	256.5
2 Main TS	82.18	172.5	257.1
3 Main TS	82.61	173.9	258.0
4 Main TS	83.13	175.9	259.4
5 Main TS	83.77	178.7	261.4
6 Main TS	84.62	182.1	264.2
7 Main TS	86.09	183.2	267.6
8 Main TS	90.81	166.5	268.7
9 Main TS	106.7	132.9	252.0
10 Main TS	127.3	213.1	218.4
11 Main TS	149.4	219.6	198.6
12 Main TS	153.1	221.6	205.1
13 Main TS	153.7	221.8	207.1
14 Main TS	154.0	222.0	207.3
15 Main TS	154.3	222.1	207.5
16 Main TS	154.6	222.2	207.6
17 Main TS	154.9	222.3	207.7

Remarks:

* Specified by user.

HYSYS Column Specsheet — Senior Project Trial-dist only.hsc

Distillation Column @Main

Profile Estimates

	Temperature (C)	Net Liquid (kgmole/h)	Net Vapour (kgmole/h)
18 Main TS	155.2	222.4	207.8
19 Main TS	155.5	222.5	207.9
20 Main TS	155.7	221.7	208.0
Reboiler	158.0	14.50	207.2

Stage Efficiencies

Stages	Overall Efficiency	A*	B*	R*	S*	
Condenser	1.000	1.000	1.000	1.000	1.000	
1 Main TS	1.000	1.000	1.000	1.000	1.000	
2 Main TS	1.000	1.000	1.000	1.000	1.000	
3 Main TS	1.000	1.000	1.000	1.000	1.000	
4 Main TS	1.000	1.000	1.000	1.000	1.000	
5 Main TS	1.000	1.000	1.000	1.000	1.000	
6 Main TS	1.000	1.000	1.000	1.000	1.000	
7 Main TS	1.000	1.000	1.000	1.000	1.000	
8 Main TS	1.000	1.000	1.000	1.000	1.000	
9 Main TS	1.000	1.000	1.000	1.000	1.000	
10 Main TS	1.000	1.000	1.000	1.000	1.000	
11 Main TS	1.000	1.000	1.000	1.000	1.000	
12 Main TS	1.000	1.000	1.000	1.000	1.000	
13 Main TS	1.000	1.000	1.000	1.000	1.000	
14 Main TS	1.000	1.000	1.000	1.000	1.000	
15 Main TS	1.000	1.000	1.000	1.000	1.000	
16 Main TS	1.000	1.000	1.000	1.000	1.000	
17 Main TS	1.000	1.000	1.000	1.000	1.000	
18 Main TS	1.000	1.000	1.000	1.000	1.000	
19 Main TS	1.000	1.000	1.000	1.000	1.000	
20 Main TS	1.000	1.000	1.000	1.000	1.000	
Reboiler	1.000	1.000	1.000	1.000	1.000	

Properties : 1

	Overall	Liquid Phase			
Vapour/Phase Fraction	0.0000	1.000			
Temperature: (C)	25.00	25.00			
Pressure: (kPa)	120.0	120.0			
Molar Flow (kgmole/h)	100.0	100.0			
Mass Flow (kg/h)	2479.	2479.			
Liquid Volume Flow (m3/h)	2.484	2.484			
Molar Enthalpy (kJ/kgmole)	-3.100e+05	-3.100e+05			
Mass Enthalpy (kJ/kg)	-1.250e+04	-1.250e+04			
Molar Entropy (kJ/kgmole-C)	128.2	128.2			
Mass Entropy (kJ/kg-C)	5.172	5.172			
Heat Flow (kJ/h)	-3.100e+07	-3.100e+07			
Molar Density (kgmole/m3)	40.26	40.26			
Mass Density (kg/m3)	998.1	998.1			
Std Liquid Mass Density (kg/m3)	1006.	1006.			
Molar Heat Capacity (kJ/kgmole-C)	102.4	102.4			
Mass Heat Capacity (kJ/kg-C)	4.129	4.129			
ThermalConductivity (W/m-K)	0.2822	0.2822			
Viscosity (cP)	1.667	1.667			
Surface Tension (dyne/cm)	8.889	8.889			
Molecular Weight	24.79	24.79			
Z Factor	0.001203	0.001203			

Remarks:

* Specified by user.

HYSYS Column Specsheet — Senior Project Trial-dist only.hsc

Distillation Column @Main

Properties : 2

	Overall	Liquid Phase			
Vapour/Phase Fraction	0.0000	1.000			
Temperature: (C)	81.72	81.72			
Pressure: (kPa)	107.0	107.0			
Molar Flow (kgmole/h)	85.50	85.50			
Mass Flow (kg/h)	1553.	1553.			
Liquid Volume Flow (m3/h)	1.556	1.556			
Molar Enthalpy (kJ/kgmole)	-2.802e+05	-2.802e+05			
Mass Enthalpy (kJ/kg)	-1.542e+04	-1.542e+04			
Molar Entropy (kJ/kgmole-C)	103.5	103.5			
Mass Entropy (kJ/kg-C)	5.696	5.696			
Heat Flow (kJ/h)	-2.395e+07	-2.395e+07			
Molar Density (kgmole/m3)	52.82	52.82			
Mass Density (kg/m3)	959.6	959.6			
Std Liquid Mass Density (kg/m3)	1012.	1012.			
Molar Heat Capacity (kJ/kgmole-C)	86.95	86.95			
Mass Heat Capacity (kJ/kg-C)	4.786	4.786			
ThermalConductivity (W/m-K)	0.2685	0.2685			
Viscosity (cP)	0.3536	0.3536			
Surface Tension (dyne/cm)	2.411	2.411			
Molecular Weight	18.17	18.17			
Z Factor	0.0006866	0.0006866			

Properties : 3

	Overall	Liquid Phase			
Vapour/Phase Fraction	0.0000	1.000			
Temperature: (C)	158.0	158.0			
Pressure: (kPa)	127.0	127.0			
Molar Flow (kgmole/h)	14.50	14.50			
Mass Flow (kg/h)	926.0	926.0			
Liquid Volume Flow (m3/h)	0.9279	0.9279			
Molar Enthalpy (kJ/kgmole)	-4.316e+05	-4.316e+05			
Mass Enthalpy (kJ/kg)	-6758.	-6758.			
Molar Entropy (kJ/kgmole-C)	602.2	602.2			
Mass Entropy (kJ/kg-C)	9.429	9.429			
Heat Flow (kJ/h)	-6.258e+06	-6.258e+06			
Molar Density (kgmole/m3)	15.79	15.79			
Mass Density (kg/m3)	1008.	1008.			
Std Liquid Mass Density (kg/m3)	1201.	1201.			
Molar Heat Capacity (kJ/kgmole-C)	192.7	192.7			
Mass Heat Capacity (kJ/kg-C)	3.017	3.017			
ThermalConductivity (W/m-K)	0.1691	0.1691			
Viscosity (cP)	0.5710	0.5710			
Surface Tension (dyne/cm)	27.07	27.07			
Molecular Weight	63.86	63.86			
Z Factor	0.002244	0.002244			

Remarks:

* Specified by user.

Appendix E: HYSYS CSTR Results

HYSYS CSTR Specsheet — Senior Project Version 3 with reactor.hsc

CSTR Reactor

Inlet		Outlet		Energy	
NAME	FROM OPER	NAME	TO OPER	NAME	FROM OPER
Reactor Feed	Mixer: MIX-101	Vapour Out: 1		Q-102	
		Liquid Out: Reactor Products			

Parameters

Physical Parameters		Optional Heat Transfer: Heating	
Delta P	Vessel Volume	Duty	Energy Stream
0.0000 kPa *	2.000 m3 *	2.000e+05 kJ/h *	Q-102

Reactor Results Summary for : Global Rxn Set

	Act. % Conv.	Base Comp.	Rxn Extent (kgmole/h)
Rxn-1	10.00	A*	10.00
Rxn-2	100.0	B*	5.000

Reactions Information

Reaction: Rxn-1

Component	Mole Weight	Stoichiometric Coeff.
A*	18.02	-1.000 *
B*	44.05	-1.000 *
R*	62.07	1.000 *

Reaction: Rxn-2

Component	Mole Weight	Stoichiometric Coeff.
B*	44.05	-2.000 *
S*	88.11	1.000 *

Reaction Component Summary

	Total Inflow (kgmole/h)	Total Rxn (kgmole/h)	Total Outflow (kgmole/h)
A*	100.0	-10.00	90.00
B*	10.00	-10.00	3.418e-07
R*	0.0000	10.00	10.00
S*	0.0000	1.100e-05	1.100e-05

Properties : Reactor Feed

	Overall	Liquid Phase			
Vapour/Phase Fraction	0.0000	1.000			
Temperature: (C)	25.00	25.00			
Pressure: (kPa)	101.0	101.0			
Molar Flow (kgmole/h)	110.0	110.0			
Mass Flow (kg/h)	2242.	2242.			
Liquid Volume Flow (m3/h)	2.247	2.247			
Molar Enthalpy (kJ/kgmole)	-2.770e+05	-2.770e+05			
Mass Enthalpy (kJ/kg)	-1.359e+04	-1.359e+04			
Molar Entropy (kJ/kgmole-C)	98.48	98.48			
Mass Entropy (kJ/kg-C)	4.832	4.832			
Heat Flow (kJ/h)	-3.047e+07	-3.047e+07			
Molar Density (kgmole/m3)	47.21	47.21			
Mass Density (kg/m3)	962.3	962.3			
Std Liquid Mass Density (kg/m3)	970.4	970.4			
Molar Heat Capacity (kJ/kgmole-C)	91.12	91.12			
Mass Heat Capacity (kJ/kg-C)	4.471	4.471			

Remarks:

* Specified by user.

HYSYS CSTR Specsheet — Senior Project Version 3 with reactor.hsc

CSTR Reactor

Properties : Reactor Feed

	Overall	Liquid Phase			
ThermalConductivity (W/m-K)	0.2822	0.2822			
Viscosity (cP)	0.7423	0.7423			
Surface Tension (dyne/cm)	4.694	4.694			
Molecular Weight	20.38	20.38			
Z Factor	0.0008630	0.0008630			

Properties : Reactor Products

	Overall	Liquid Phase	Vapour Phase		
Vapour/Phase Fraction	0.0000 *	1.000	0.0000		
Temperature: (C)	24.62	24.62	24.62		
Pressure: (kPa)	101.0	101.0	101.0		
Molar Flow (kgmole/h)	100.0	100.0	0.0000		
Mass Flow (kg/h)	2242.	2242.	0.0000		
Liquid Volume Flow (m3/h)	2.247	2.247	0.0000		
Molar Enthalpy (kJ/kgmole)	-3.027e+05	-3.027e+05	-2.425e+05		
Mass Enthalpy (kJ/kg)	-1.350e+04	-1.350e+04	-1.314e+04		
Molar Entropy (kJ/kgmole-C)	109.5	109.5	217.7		
Mass Entropy (kJ/kg-C)	4.882	4.882	11.80		
Heat Flow (kJ/h)	-3.027e+07	-3.027e+07	0.0000		
Molar Density (kgmole/m3)	44.66	44.66	0.04080		
Mass Density (kg/m3)	1001.	1001.	0.7528		
Std Liquid Mass Density (kg/m3)	1009.	1009.	1014.		
Molar Heat Capacity (kJ/kgmole-C)	98.53	98.53	34.39		
Mass Heat Capacity (kJ/kg-C)	4.395	4.395	1.864		
ThermalConductivity (W/m-K)	0.2879	0.2879	0.02223		
Viscosity (cP)	1.498	1.498	0.007154		
Surface Tension (dyne/cm)	6.985	6.985	---		
Molecular Weight	22.42	22.42	18.45		
Z Factor	0.0009135	0.0009135	1.000		

Properties : 1

	Overall	Liquid Phase	Vapour Phase		
Vapour/Phase Fraction	1.000	0.0000	1.000		
Temperature: (C)	24.62	24.62	24.62		
Pressure: (kPa)	101.0	101.0	101.0		
Molar Flow (kgmole/h)	0.0000	0.0000	0.0000		
Mass Flow (kg/h)	0.0000	0.0000	0.0000		
Liquid Volume Flow (m3/h)	0.0000	0.0000	0.0000		
Molar Enthalpy (kJ/kgmole)	-2.425e+05	-3.027e+05	-2.425e+05		
Mass Enthalpy (kJ/kg)	-1.314e+04	-1.350e+04	-1.314e+04		
Molar Entropy (kJ/kgmole-C)	217.7	109.5	217.7		
Mass Entropy (kJ/kg-C)	11.80	4.882	11.80		
Heat Flow (kJ/h)	0.0000	0.0000	0.0000		
Molar Density (kgmole/m3)	0.04080	44.66	0.04080		
Mass Density (kg/m3)	0.7528	1001.	0.7528		
Std Liquid Mass Density (kg/m3)	---	1009.	1014.		
Molar Heat Capacity (kJ/kgmole-C)	34.39	98.53	34.39		
Mass Heat Capacity (kJ/kg-C)	1.864	4.395	1.864		
ThermalConductivity (W/m-K)	0.02223	0.2879	0.02223		
Viscosity (cP)	0.007154	1.498	0.007154		
Surface Tension (dyne/cm)	---	6.985	---		
Molecular Weight	18.45	22.42	18.45		
Z Factor	1.000	0.0009135	1.000		

Remarks:

* Specified by user.

HYSYS Column Specsheet Senior Project Basic Plant Final Version.hsc

Distillation Column @Main

Inlet			Outlet		
NAME	STAGE	FROM OPER	NAME	STAGE	TO OPER
Q-101	Reboiler		Q-100	Condenser	
Reactor Products	10 Main TS	Cont. Stirred Tank Reactor	2	Condenser	Recycle: RCY-1
			3	Reboiler	
			** New **		

General Parameters

Sub-Flow Sheet:	Distillation Column (COL1)	Number of Stages:	20 *

Column Solving Algorithm: Modified HYSIM Inside-Out

Solving Options		Acceleration Parameters	
Maximum Iterations:	5000. *	Accelerate K Value & H Model Parameters:	Off
Equilibrium Error Tolerance:	1.000e-05 *		
Heat/Spec Error Tolerance:	0.0005000 *		
Save Solutions as Initial Estimate:	On		
Super Critical Handling Model:	Simple K		
Trace Level:	Low		
Init from Ideal K's:	Off	Damping Parameters	
Initial Estimate Generator Parameters		Azeotrope Check:	Off
Iterative IEG (Good for Chemicals):	Off	Adaptive Initial Damping Factor:	0.1339 *
		Adaptive Damping Period:	10
		Update Initial Damping Factor:	Off

Specifications Summary

	Specified Value	Current Value	Wt. Error	Wt. Tol.	Abs. Tol.	Active	Estimate
Reflux Ratio	2.000 *	2.000	3.843e-05	0.01000 *	0.01000 *	On	On
Comp Fraction A in Con	0.9999 *	0.9999	4.223e-07	0.01000 *	0.001000 *	On	On
Distillate Rate	200.0 kgmole/h *	200.0 kgmole/h	0.0000	0.01000 *	1.000 kgmole/h *	Off	On
Reflux Rate	400.0 kgmole/h *	400.0 kgmole/h	0.0001020	0.01000 *	1.000 kgmole/h *	Off	On
Duty Q-100 Cond	-2.500e+07 kJ/h *	-2.500e+07 kJ/h	1.949e-07	0.01000 *	10.00 kJ/h *	Off	On
Btms Prod Rate	70.00 kgmole/h *	70.00 kgmole/h	0.0000	0.01000 *	1.000 kgmole/h *	Off	On
Duty Q-101 Reboiler	2.650e+07 kJ/h *	2.648e+07 kJ/h	-7.211e-06	0.01000 *	10.00 kJ/h *	Off	On
Comp Fraction R in Reb	1.000 *	1.000	-0.1020	0.01000 *	0.001000 *	Off	On

Column Specification Details

Reflux Ratio

Stage:	Condenser	Flow Basis:	Molar	Liquid Specification:	Light

Comp Fraction A in Cond

Stage:	Condenser	Flow Basis:	Mole Fraction	Phase:	Liquid
Components:		A*			

Distillate Rate

Stream:	2	Flow Basis:	Molar

Reflux Rate

Stage:	Condenser	Flow Basis:	Molar	Liquid Specification:	Light

Duty Q-100 Cond

Energy Stream:	Q-100

Btms Prod Rate

Stream:	3	Flow Basis:	Molar

Remarks:

* Specified by user.

HYSYS Column Specsheet Senior Project Basic Plant Final Version.hsc

Distillation Column @Main

Column Specification Details

Duty Q-101 Reboiler

Energy Stream:	Q-101				

Comp Fraction R in Reb

Stage:	Reboiler	Flow Basis:	Mole Fraction	Phase:	Liquid

Components:	R*				

Sub-Flowsheet

Feed Streams			Product Streams		
Internal Stream	External Stream	Transfer Basis	Internal Stream	External Stream	Transfer Basis
Q-101	Reboiler Duty @Main	None Req'd	Q-100	Condenser Duty @Main	None Req'd
Reactor Products	r Products/Distillation Feed @	T-P Flash	2	Recycle Stream @Main	T-P Flash
			3	Product Stream @Main	T-P Flash
			** New **		

Tray Summary

Flow Basis:	Molar	Reflux Ratio:	2.000

	Temp. (C)	Pressure (kPa)	Liquid (kgmole/h)	Vapour (kgmole/h)	Feeds (kgmole/h)		Draws (kgmole/h)		Duties (kJ/h)
Condenser	81.64	107.0	400.0	---	---	Q	200.0	L	-2.500e+07
1 Main TS	81.67	107.0	399.7	600.1					---
2 Main TS	82.07	108.1	397.5	599.7					---
3 Main TS	83.70	109.1	382.5	597.6					---
4 Main TS	92.59	110.2	328.1	582.5					---
5 Main TS	115.4	111.2	290.5	528.1					---
6 Main TS	130.8	112.3	291.2	490.6					---
7 Main TS	134.7	113.3	292.7	491.2					---
8 Main TS	135.5	114.4	293.0	492.7					---
9 Main TS	135.9	115.4	293.2	493.0					---
10 Main TS	136.2	116.5	529.4	493.2	270.0	L			---
11 Main TS	150.9	117.5	545.9	459.4					---
12 Main TS	153.1	118.6	549.0	476.0					---
13 Main TS	153.6	119.6	549.5	479.0					---
14 Main TS	153.9	120.7	549.8	479.5					---
15 Main TS	154.2	121.7	550.1	479.8					---
16 Main TS	154.5	122.8	550.4	480.1					---
17 Main TS	154.7	123.8	550.6	480.4					---
18 Main TS	155.0	124.9	550.9	480.7					---
19 Main TS	155.3	125.9	551.2	480.9					---
20 Main TS	155.6	127.0	551.8	481.2					---
Reboiler	155.6	127.0	---	481.8	---	Q	70.00	L	2.648e+07

Profile Estimates

	Temperature (C)	Net Liquid (kgmole/h)	Net Vapour (kgmole/h)
Condenser	81.64	600.1	1.217e-19
1 Main TS	81.67	399.7	600.1
2 Main TS	82.07	397.5	599.7
3 Main TS	83.70	382.5	597.6
4 Main TS	92.59	328.1	582.5
5 Main TS	115.4	290.5	528.1
6 Main TS	130.8	291.2	490.6
7 Main TS	134.7	292.7	491.2

Remarks:

* Specified by user.

HYSYS Column Specsheet Senior Project Basic Plant Final Version.hsc

Distillation Column @Main

Profile Estimates

	Temperature (C)	Net Liquid (kgmole/h)	Net Vapour (kgmole/h)
8 Main TS	135.5	293.0	492.7
9 Main TS	135.9	293.2	493.0
10 Main TS	136.2	529.4	493.2
11 Main TS	150.9	545.9	459.4
12 Main TS	153.1	549.0	476.0
13 Main TS	153.6	549.5	479.0
14 Main TS	153.9	549.8	479.5
15 Main TS	154.2	550.1	479.8
16 Main TS	154.5	550.4	480.1
17 Main TS	154.7	550.6	480.4
18 Main TS	155.0	550.9	480.7
19 Main TS	155.3	551.2	480.9
20 Main TS	155.6	551.8	481.2
Reboiler	155.6	70.00	481.8

Stage Efficiencies

Stages	Overall Efficiency	A*	B*	R*	S*	
Condenser	1.000	1.000	1.000	1.000	1.000	
1 Main TS	1.000	1.000	1.000	1.000	1.000	
2 Main TS	1.000	1.000	1.000	1.000	1.000	
3 Main TS	1.000	1.000	1.000	1.000	1.000	
4 Main TS	1.000	1.000	1.000	1.000	1.000	
5 Main TS	1.000	1.000	1.000	1.000	1.000	
6 Main TS	1.000	1.000	1.000	1.000	1.000	
7 Main TS	1.000	1.000	1.000	1.000	1.000	
8 Main TS	1.000	1.000	1.000	1.000	1.000	
9 Main TS	1.000	1.000	1.000	1.000	1.000	
10 Main TS	1.000	1.000	1.000	1.000	1.000	
11 Main TS	1.000	1.000	1.000	1.000	1.000	
12 Main TS	1.000	1.000	1.000	1.000	1.000	
13 Main TS	1.000	1.000	1.000	1.000	1.000	
14 Main TS	1.000	1.000	1.000	1.000	1.000	
15 Main TS	1.000	1.000	1.000	1.000	1.000	
16 Main TS	1.000	1.000	1.000	1.000	1.000	
17 Main TS	1.000	1.000	1.000	1.000	1.000	
18 Main TS	1.000	1.000	1.000	1.000	1.000	
19 Main TS	1.000	1.000	1.000	1.000	1.000	
20 Main TS	1.000	1.000	1.000	1.000	1.000	
Reboiler	1.000	1.000	1.000	1.000	1.000	

Properties : Reactor Products

		Overall	Liquid Phase			
Vapour/Phase Fraction		0.0000	1.000			
Temperature:	(C)	67.47	67.47			
Pressure:	(kPa)	101.0	101.0			
Molar Flow	(kgmole/h)	270.0	270.0			
Mass Flow	(kg/h)	7949.	7949.			
Liquid Volume Flow	(m3/h)	7.965	7.965			
Molar Enthalpy	(kJ/kgmole)	-3.247e+05	-3.247e+05			
Mass Enthalpy	(kJ/kg)	-1.103e+04	-1.103e+04			
Molar Entropy	(kJ/kgmole-C)	219.1	219.1			
Mass Entropy	(kJ/kg-C)	7.444	7.444			
Heat Flow	(kJ/h)	-8.768e+07	-8.768e+07			

Remarks:

* Specified by user.

HYSYS Column Specsheet Senior Project Basic Plant Final Version.hsc

Distillation Column @Main

Properties : Reactor Products

	Overall	Liquid Phase			
Molar Density (kgmole/m3)	32.93	32.93			
Mass Density (kg/m3)	969.3	969.3			
Std Liquid Mass Density (kg/m3)	1015.	1015.			
Molar Heat Capacity (kJ/kgmole-C)	115.7	115.7			
Mass Heat Capacity (kJ/kg-C)	3.932	3.932			
ThermalConductivity (W/m-K)	0.2560	0.2560			
Viscosity (cP)	1.111	1.111			
Surface Tension (dyne/cm)	12.02	12.02			
Molecular Weight	29.44	29.44			
Z Factor	0.001083	0.001083			

Properties : 2

	Overall	Liquid Phase			
Vapour/Phase Fraction	0.0000	1.000			
Temperature: (C)	81.64	81.64			
Pressure: (kPa)	107.0	107.0			
Molar Flow (kgmole/h)	200.0	200.0			
Mass Flow (kg/h)	3604.	3604.			
Liquid Volume Flow (m3/h)	3.611	3.611			
Molar Enthalpy (kJ/kgmole)	-2.808e+05	-2.808e+05			
Mass Enthalpy (kJ/kg)	-1.558e+04	-1.558e+04			
Molar Entropy (kJ/kgmole-C)	101.0	101.0			
Mass Entropy (kJ/kg-C)	5.607	5.607			
Heat Flow (kJ/h)	-5.616e+07	-5.616e+07			
Molar Density (kgmole/m3)	53.45	53.45			
Mass Density (kg/m3)	963.1	963.1			
Std Liquid Mass Density (kg/m3)	1015.	1015.			
Molar Heat Capacity (kJ/kgmole-C)	86.68	86.68			
Mass Heat Capacity (kJ/kg-C)	4.810	4.810			
ThermalConductivity (W/m-K)	0.2695	0.2695			
Viscosity (cP)	0.3577	0.3577			
Surface Tension (dyne/cm)	2.343	2.343			
Molecular Weight	18.02	18.02			
Z Factor	0.0006787	0.0006787			

Properties : 3

	Overall	Liquid Phase			
Vapour/Phase Fraction	0.0000	1.000			
Temperature: (C)	155.6	155.6			
Pressure: (kPa)	127.0	127.0			
Molar Flow (kgmole/h)	70.00	70.00			
Mass Flow (kg/h)	4345.	4345.			
Liquid Volume Flow (m3/h)	4.353	4.353			
Molar Enthalpy (kJ/kgmole)	-4.292e+05	-4.292e+05			
Mass Enthalpy (kJ/kg)	-6915.	-6915.			
Molar Entropy (kJ/kgmole-C)	647.1	647.1			
Mass Entropy (kJ/kg-C)	10.43	10.43			
Heat Flow (kJ/h)	-3.004e+07	-3.004e+07			
Molar Density (kgmole/m3)	16.71	16.71			
Mass Density (kg/m3)	1037.	1037.			
Std Liquid Mass Density (kg/m3)	1228.	1228.			
Molar Heat Capacity (kJ/kgmole-C)	201.2	201.2			
Mass Heat Capacity (kJ/kg-C)	3.242	3.242			
ThermalConductivity (W/m-K)	0.1759	0.1759			

Remarks:

* Specified by user.

HYSYS Column Specsheet Senior Project Basic Plant Final Version.hsc

Distillation Column @Main

Properties : 3

		Overall	Liquid Phase			
Viscosity	(cP)	0.6801	0.6801			
Surface Tension	(dyne/cm)	28.45	28.45			
Molecular Weight		62.07	62.07			
Z Factor		0.002132	0.002132			

Remarks:

* Specified by user.

HYSYS CSTR Specsheet Senior Project Basic Plant Final Version.hsc

CSTR Reactor

Inlet		Outlet		Energy	
NAME	FROM OPER	NAME	TO OPER	NAME	FROM OPER
Reactor Feed	Mixer: MIX-101	Vapour Out: 1		Reactor Duty	
		Liquid Out: r Products/Distillation	Column Distillation Column		

Parameters

Physical Parameters		Optional Heat Transfer: Heating	
Delta P	**Vessel Volume**	**Duty**	**Energy Stream**
0.0000 kPa *	2.000 m3 *	1.750e+06 kJ/h *	Reactor Duty

Reactor Results Summary for : Global Rxn Set

	Act. % Conv.	Base Comp.	Rxn Extent (kgmole/h)
Rxn-1	100.0	B*	70.00
Rxn-2	100.0	B*	35.00

Reactions Information

Reaction: Rxn-1

Component	Mole Weight	Stoichiometric Coeff.
A*	18.02	-1.000 *
B*	44.05	-1.000 *
R*	62.07	1.000 *

Reaction: Rxn-2

Component	Mole Weight	Stoichiometric Coeff.
B*	44.05	-2.000 *
S*	88.11	1.000 *

Reaction Component Summary

	Total Inflow (kgmole/h)	Total Rxn (kgmole/h)	Total Outflow (kgmole/h)
A*	270.0	-69.99	200.0
B*	70.00	-70.00	7.998e-06
R*	0.01999	70.00	70.02
S*	6.364e-29	0.002516	0.002516

Properties : Reactor Feed

		Overall	Liquid Phase			
Vapour/Phase Fraction		0.0000	1.000			
Temperature:	(C)	55.79	55.79			
Pressure:	(kPa)	101.0	101.0			
Molar Flow	(kgmole/h)	340.0	340.0			
Mass Flow	(kg/h)	7949.	7949.			
Liquid Volume Flow	(m3/h)	7.965	7.965			
Molar Enthalpy	(kJ/kgmole)	-2.630e+05	-2.630e+05			
Mass Enthalpy	(kJ/kg)	-1.125e+04	-1.125e+04			
Molar Entropy	(kJ/kgmole-C)	164.8	164.8			
Mass Entropy	(kJ/kg-C)	7.050	7.050			
Heat Flow	(kJ/h)	-8.943e+07	-8.943e+07			
Molar Density	(kgmole/m3)	38.02	38.02			
Mass Density	(kg/m3)	888.8	888.8			
Std Liquid Mass Density	(kg/m3)	925.9	925.9			
Molar Heat Capacity	(kJ/kgmole-C)	96.05	96.05			
Mass Heat Capacity	(kJ/kg-C)	4.109	4.109			

Remarks:

* Specified by user.

HYSYS CSTR Specsheet Senior Project Basic Plant Final Version.hsc

CSTR Reactor

Properties : Reactor Feed

	Overall	Liquid Phase			
ThermalConductivity (W/m-K)	0.2495	0.2495			
Viscosity (cP)	0.3703	0.3703			
Surface Tension (dyne/cm)	5.898	5.898			
Molecular Weight	23.38	23.38			
Z Factor	0.0009714	0.0009714			

Properties : Reactor Products/Distillation Feed

	Overall	Liquid Phase	Vapour Phase		
Vapour/Phase Fraction	0.0000 *	1.000	0.0000		
Temperature: (C)	67.47	67.47	67.47		
Pressure: (kPa)	101.0	101.0	101.0		
Molar Flow (kgmole/h)	270.0	270.0	0.0000		
Mass Flow (kg/h)	7949.	7949.	0.0000		
Liquid Volume Flow (m3/h)	7.965	7.965	0.0000		
Molar Enthalpy (kJ/kgmole)	-3.247e+05	-3.247e+05	-2.437e+05		
Mass Enthalpy (kJ/kg)	-1.103e+04	-1.103e+04	-1.264e+04		
Molar Entropy (kJ/kgmole-C)	219.1	219.1	232.8		
Mass Entropy (kJ/kg-C)	7.444	7.444	12.08		
Heat Flow (kJ/h)	-8.768e+07	-8.768e+07	0.0000		
Molar Density (kgmole/m3)	32.93	32.93	0.03566		
Mass Density (kg/m3)	969.3	969.3	0.6875		
Std Liquid Mass Density (kg/m3)	1015.	1015.	1012.		
Molar Heat Capacity (kJ/kgmole-C)	115.7	115.7	36.21		
Mass Heat Capacity (kJ/kg-C)	3.932	3.932	1.879		
ThermalConductivity (W/m-K)	0.2560	0.2560	0.02538		
Viscosity (cP)	1.111	1.111	0.008326		
Surface Tension (dyne/cm)	12.02	12.02	---		
Molecular Weight	29.44	29.44	19.28		
Z Factor	0.001083	0.001083	1.000		

Properties : 1

	Overall	Liquid Phase	Vapour Phase		
Vapour/Phase Fraction	1.000	0.0000	1.000		
Temperature: (C)	67.47	67.47	67.47		
Pressure: (kPa)	101.0	101.0	101.0		
Molar Flow (kgmole/h)	0.0000	0.0000	0.0000		
Mass Flow (kg/h)	0.0000	0.0000	0.0000		
Liquid Volume Flow (m3/h)	0.0000	0.0000	0.0000		
Molar Enthalpy (kJ/kgmole)	-2.437e+05	-3.247e+05	-2.437e+05		
Mass Enthalpy (kJ/kg)	-1.264e+04	-1.103e+04	-1.264e+04		
Molar Entropy (kJ/kgmole-C)	232.8	219.1	232.8		
Mass Entropy (kJ/kg-C)	12.08	7.444	12.08		
Heat Flow (kJ/h)	0.0000	0.0000	0.0000		
Molar Density (kgmole/m3)	0.03566	32.93	0.03566		
Mass Density (kg/m3)	0.6875	969.3	0.6875		
Std Liquid Mass Density (kg/m3)	---	1015.	1012.		
Molar Heat Capacity (kJ/kgmole-C)	36.21	115.7	36.21		
Mass Heat Capacity (kJ/kg-C)	1.879	3.932	1.879		
ThermalConductivity (W/m-K)	0.02538	0.2560	0.02538		
Viscosity (cP)	0.008326	1.111	0.008326		
Surface Tension (dyne/cm)	---	12.02	---		
Molecular Weight	19.28	29.44	19.28		
Z Factor	1.000	0.001083	1.000		

Remarks:

* Specified by user.

HYSYS Controller Specsheet Senior Project Version 11 dist control.hsc

Distillation Column Temperature Controller

Process Variable		Output	Cascade
OBJECT	VARIABLE	OBJECT	OBJECT
Column Distillation Column	ge Temperature (5__Main TS	Energy Stream: Reboiler Duty	

Configuration

Minimun:	80.00 C *	Maximum:	180.0 C *	Control Action:	Reverse

Operational Parameters

SP:	130.5 C *	PV:	135.5 C	OP:	75.37	Controller Mode:	Auto

Tuning

Kp:	1.500 *	Ti:	30.00 minutes *	Td:	0.0000 minutes *

Ramping

Target SP:	---	Ramp Duration:	---

Control Valve Parameters

Duty Valve Source:	Direct Q	SP:	---	Min. Duty Avail:	0.0000 kJ/h *	Max. Duty Avail:	8.000e+07 kJ/h *

Remarks:

Date:	Fri May 05 10:50:02 2000	Version:	HYSYS v1.5.2 (Build 1706)	Page No:	1	Of:	1

* Specified by user.

HYSYS Controller Specsheet Senior Project Version 11 dist control.hsc

Tank Temperature Controller

Process Variable		Output	Cascade
OBJECT	VARIABLE	OBJECT	OBJECT
Tank: Hold Up Tank	Vessel Temperature	Energy Stream: Tank Duty	

Configuration

Minimun:	30.00 C *	Maximum:	120.0 C *	Control Action:	Reverse

Operational Parameters

SP:	70.00 C *	PV:	69.78 C	OP:	42.34	Controller Mode:	Auto

Tuning

Kp:	1.500 *	Ti:	60.00 minutes *	Td:	0.0000 minutes *

Ramping

Target SP:	---	Ramp Duration:	---

Control Valve Parameters

Duty Valve Source:	Direct Q	SP:	-2.870e+06 kJ/h	Min. Duty Avail:	-5.000e+06 kJ/h *	Max. Duty Avail:	3.000e+04 kJ/h *

Remarks:

* Specified by user.

HYSYS Controller Specsheet Senior Project Version 10 dist control.hsc

Ratio Controller

Process Variable		Output	Cascade
OBJECT	VARIABLE	OBJECT	OBJECT
SpreadsheetSPRDSHT-1	B5: A Ratio	Material Stream A Removal @COL1	

Configuration

Minimun:	0.0000 *	Maximum:	2.000 *	Control Action:	Direct

Operational Parameters

SP:	1.000 *	PV:	1.000	OP:	50.00	Controller Mode:	Auto

Tuning

Kp:	1.000 *	Ti:	30.00 minutes *	Td:	0.0000 minutes *

Ramping

Target SP:	---	Ramp Duration:	---

Control Valve Parameters

Actual Mol Flow:	5.000 kgmole/h	Actual Mass Flow:	101.0 kg/h	Liq Vol Flow:	0.1012 m3/h
Flow Type:	MolarFlow	Min Flow:	0.0000 kgmole/h *	Max Flow:	10.00 kgmole/h *

Remarks:

Date:	Fri May 05 12:37:51 2000	Version:	HYSYS v1.5.2 (Build 1706)	Page No:	1	Of:	1

* Specified by user.